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Dakota Sensitivity Analysis and Uncertainty Quantification, with Examples





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Dakota Uncertainty Quantification (UQ)



- UQ goals and examples
- Select Dakota examples for UQ:
 - Monte Carlo sampling
 - Local and global reliability
 - Polynomial chaos expansions / stochastic collocation
 - Mixed aleatory-epistemic approaches
 - Probabilistic design
- Dakota primarily focuses on forward propagation
 - Secondarily on estimating parameter uncertainty given data
 - Not on processing experimental data to calculate uncertainties

Drivers for Dakota UQ



Current Dakota research and development largely focuses on efficient UQ for large-scale engineering analyses.

DOE in general, ASC V&V in particular, are:

- Responding to shift from test-based to modeling and simulation-based design and certification
- Demanding risk-informed decision-making using credible M&S:
 - Predictive simulations: verified, validated for application domain of interest
 - Quantified margins and uncertainties: random variability effect is understood, best estimate with uncertainty prediction for decision-making

Why Perform Uncertainty Quantification?

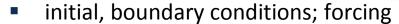


- What? Determine variability, distributions, statistics of code outputs, given uncertainty in input factors
- Why? Assess likelihood of typical or extreme outcomes. Given input uncertainty...
 - Determine mean or median performance of a system
 - Assess variability in model response
 - Find probability of reaching failure/success criteria (reliability metrics)
 - Assess range/intervals of possible outcomes
- Assess how close uncertainty-endowed code predictions are to
 - Experimental data (validation, is model sufficient for the intended application?)
 - Performance expectations or limits (quantification of margins and uncertainties; QMU)

Many Potential Uncertainties in Simulation and Validation

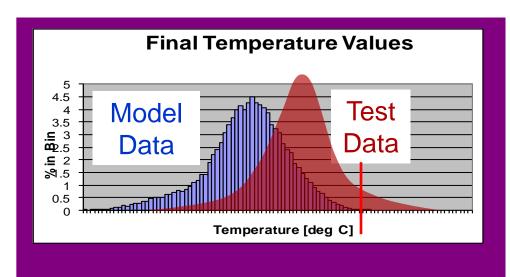


- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- material properties
- manufacturing quality
- operating environment, interference



- geometry / structure / connectivity
- experimental error (measurement error, measurement bias)
- numerical accuracy (mesh, solvers); approximation error
- human reliability, subjective judgment, linguistic imprecision

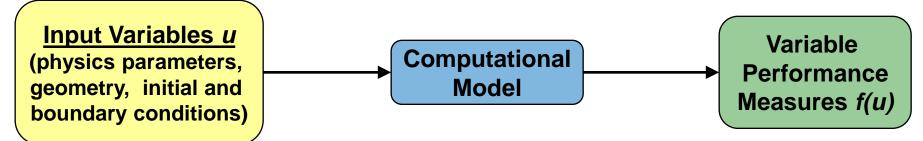
The effect of these on model outputs should be integral to an analyst's deliverable: best estimate PLUS uncertainty!



Forward Parametric Uncertainty Quantification

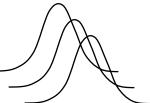


- Identify and characterize uncertain variables (may not be normal, uniform)
- Forward propagate: quantify the effect that (potentially correlated) uncertain (nondeterministic) input variables have on model output:



Uncertainties on inputs

 Parameterized distributions: normal, uniform, gumbel, etc.



Intervals

- Means, standard deviations
- PDF, CDF from data
- Intervals
- Belief structures



Uncertainties on outputs

- Means, standard deviations
- **Probabilities**
- Reliabilities
- PDF, CDF
- **Intervals**
- Belief, plausibility



Example:

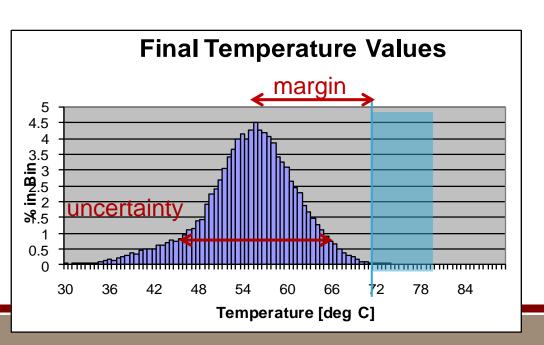
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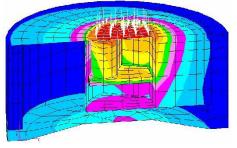
Thermal Uncertainty Quantification

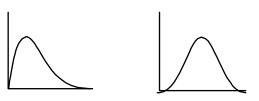
- Device subject to heating (experiment or computational simulation)
- Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by

$$u_1, ..., u_N$$

• Response temperature $f(u)=T(u_1, ..., u_N)$ calculated by heat transfer code







Given distributions of $u_1,...,u_N$, UQ methods calculate statistical info on outputs:

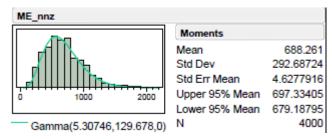
- Mean(T), StdDev(T), Probability($T \ge T_{\text{critical}}$)
- Probability distribution of temperatures
- Correlations (trends) and sensitivity of temperature

Example: Uncertainty in Boiling Rate in Nuclear Reactor Core

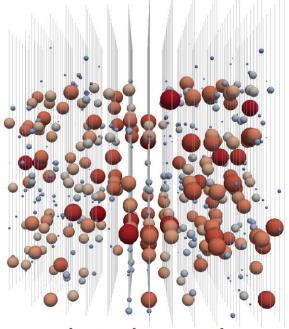


	ME_nnz		ME_meannz		ME_max	
	Mean	Std	Mean	Std	Mean	Std
Method		Dev		Dev		Dev
LHS (40)	651.225	297.039	127.836	27.723	361.204	55.862
LHS (400)	647.33	286.146	127.796	25.779	361.581	51.874
LHS (4000)	688.261	292.687	129.175	25.450	364.317	50.884
PCE (Θ(2))	687.875	288.140	129.151	25.7015	364.366	50.315
PCE (Θ (3))	688.083	292.974	129.231	25.3989	364.310	50.869
PCE (Θ (4))	688.099	292.808	129.213	25.4491	364.313	50.872

mean and standard deviation of key metrics



normally distributed inputs need not give rise to normal outputs...



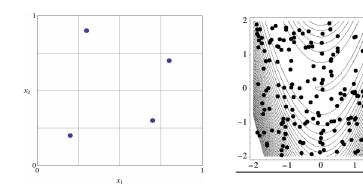
anisotropic uncertainty distribution in boiling rate throughout quarter core model

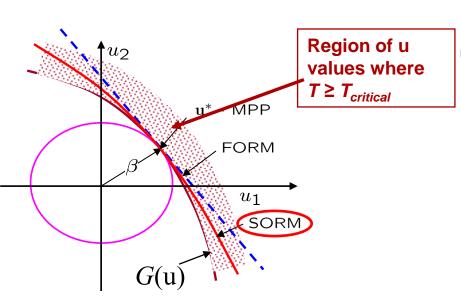




Three Core Dakota UQ Methods





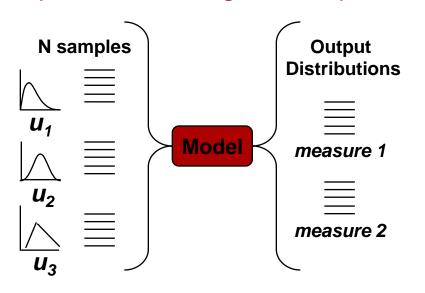


- Sampling (Monte Carlo, Latin hypercube): robust, easy to understand, slow to converge / resolve statistics
- Reliability: good at calculating probability of a particular behavior or failure / tail statistics; efficient, some methods are only local
 - Stochastic Expansions (PCE/SC global approximations): efficient tailored surrogates, statistics often derived analytically, far more efficient than sampling for reasonably smooth functions

Black-box UQ Workhorse: Random Sampling Methods



Given distributions of $u_1, ..., u_N$, sampling-based methods calculate sample statistics, e.g., on temperature $T(u_1, ..., u_N)$:



sample mean

$$\overline{T} = \frac{1}{N} \sum_{i=1}^{N} T(u^{i})$$

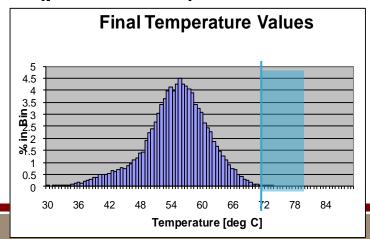
sample variance

$$T_{\sigma^2} = \frac{1}{N} \sum_{i=1}^{N} \left[T(u^i) - \overline{T} \right]^2$$

full PDF(probabilities)

- Monte Carlo sampling, Quasi-Monte Carlo
- Centroidal Voroni Tessalation (CVT)
- Latin hypercube (stratified) sampling: better convergence; stability across replicates

Robust, but slow convergence: O(N^{-1/2}), independent of dimension (in theory)



Example:





- Dakota study with LHS
- Determine mean system response, variability, margin to failure given

Density P ~ Normal(500, 30)

Young's modulusE ~ Normal(2.9e7, 2.e6)

Horizontal loadX ~ Normal(50, 3)

Vertical load
 Y ~ Normal(100, 6)

- (Dakota supports a wide range of distribution types)
- Hold width and thickness at 1.0, L at 5.
- Compute with respect to thresholds with probability_levels or response_levels
 - What is the probability(stress < 10000)?</p>
 - What is the probability(mass < 1.5)?</p>
 - What is the probability(displacement < 0.002)?</p>

Example:

Cantilever Beam UQ with Sampling



- Dakota study with LHS
- Determine mean system response, variability, margin to failure given

Density P ~ Normal(500, 30)

Young's modulusE ~ Normal(2.9e7, 2.e6)

Horizontal loadX ~ Normal(50, 3)

Vertical load
 Y ~ Normal(100, 6)

- (Dakota supports a wide range of distribution types)
- Hold width and thickness at 1.0, L at 5.
- Compute with respect to thresholds with probability_levels or response_levels
 - What is the probability(stress < 10000)? ~0.9 for uniform, 0.99 for normal</p>
 - What is the probability(mass < 1.5)? ~0.6 for uniform, 0.8 for normal</p>
 - What is the probability(displacement < 0.002)? ~0.6 for uniform, 0.7 for normal</p>

Dakota Input:

LHS Sampling for Cantilever Beam

```
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```

```
method
  sampling
  sample type lhs
  samples = 100
  seed = 3845
  num probability levels = 17 17 17
  probability levels =
   .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8 .85 .9 .95 .99 .999
   .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8 .85 .9 .95 .99 .999
   .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8 .85 .9 .95 .99 .999
  cumulative distribution
variables
  active uncertain
  continuous design = 3
    upper bounds = 1.2 \ 1.2 \ 6.0
    lower bounds = 0.8 \ 0.8 \ 4.0
                    "w"
    descriptors
                            " t."
                                    "T."
  uniform uncertain = 4
    upper bounds = 600.35.E+660.120.
    lower bounds = 400. 23.E+6 40. 80.
    descriptors
                    'p'
                          'E'
                                      'Y'
                                'X'
responses
  response functions = 3
  descriptors = 'mass' 'stress' 'displacement'
  no gradients no hessians
```

Dakota Output:

LHS Sampling for Cantilever Beam

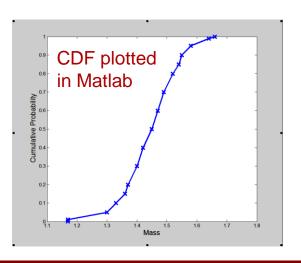


Moments and confidence intervals

```
Statistics based on 100 samples:
Moment-based statistics for each response function:
                                          Std Dev
                           Mean
                                                           Skewness
                                                                             Kurtosis
                                                                     2.5955294928e-01
               1.4460475709e+00 8.8239262134e-02 -1.6051074470e-01
        stress 8.9986343326e+04 4.0344159128e+03 6.4230716871e-02
                                                                     1.0335094626e-01
 displacement 1.9378806350e-03 1.6660999428e-04 5.5574418567e-01
                                                                     5.8860476955e-01
95% confidence intervals for each response function:
                   LowerCI Mean
                                     UpperCI Mean
                                                     LowerCI StdDev
                                                                       UpperCI StdDev
               1.4285389869e+00 1.4635561549e+00
                                                   7.7474676187e-02
                                                                     1.0250536737e-01
         mass
        stress 8.9185827682e+04 9.0786858970e+04
                                                   3.5422447886e+03
                                                                     4.6866811355e+03
              1.9048215975e-03 1.9709396725e-03
                                                   1.4628471549e-04
                                                                     1.9354670764e-04
  displacement
```

CDF (and PDF) data

```
Level mappings for each response function:
Cumulative Distribution Function (CDF) for mass:
    Response Level Probability Level Reliability Index
   1.1683297300e+00
                     1.000000000e-03
   1.1683297300e+00
                     1.000000000e-02
   1.2951111800e+00
                      5.000000000e-02
   1.3316578300e+00
                      1.000000000e-01
   1.3559746900e+00
                      1.500000000e-01
   1.3734105800e+00
                      2.000000000e-01
   1.4003385200e+00
                      3.000000000e-01
   1.4245467700e+00
                      4.000000000e-01
```



Challenge: Calculating Potentially Small Probability of Failure



- Given uncertainty in materials, geometry, and environment, how to determine likelihood of failure: $Probability(T \ge T_{critical})$?
- Perform 10,000 LHS samples and count how many exceed threshold;
 (better) perform adaptive importance sampling

Mean value: make a linearity (and possibly normality) assumption and project; great for many parameters with efficient derivatives!

$$\mu_{T} = T(\mu_{u})$$

$$\sigma_{T} = \sum_{i} \sum_{j} Cov_{u}(i, j) \frac{dg}{du_{i}}(\mu_{u}) \frac{dg}{du_{j}}(\mu_{u})$$

Reliability: directly determine input variables which give rise to failure behaviors by solving an optimization problem for a most probable point (MPP) of failure

minimize
$$u^T u$$

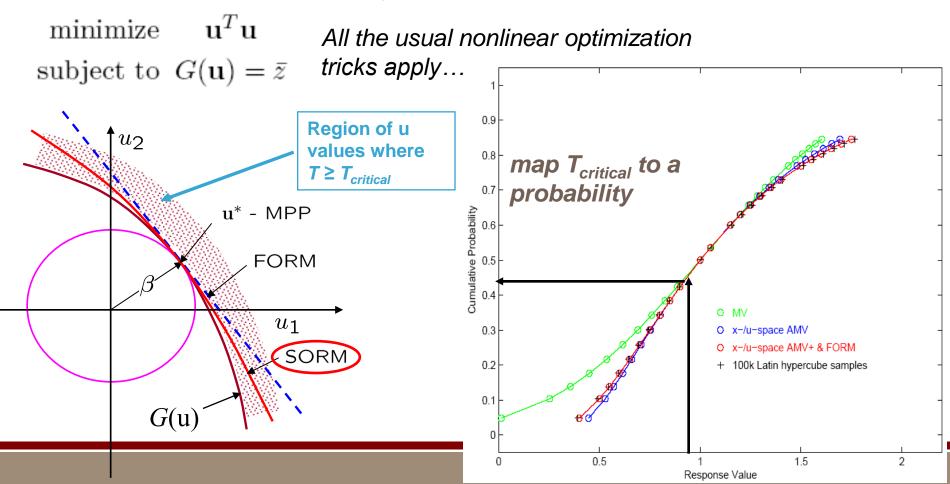
subject to $T(u) = T_{critical}$



Analytic Reliability: MPP Search

Perform optimization in uncertain variable space to determine Most Probable Point (of response or failure occurring) for G(u) = T(u).

Reliability Index Approach (RIA)



Efficient Global Reliability Analysis Using Gaussian Process Surrogate + MMAIS



- Efficient global optimization (EGO)-like approach to solve optimization problem
- Expected feasibility function: balance exploration with local search near failure boundary to refine the GP
- Cost competitive with best local MPP search methods, yet better probability of failure estimates; addresses nonlinear and multimodal challenges

Gaussian process model (level curves) of reliability limit state with 10 samples 28 samples failure region exploit safe region explore

Generalized Polynomial Chaos Expansions (PCE)



Approximate response with Galerkin projection using multivariate orthogonal polynomial basis functions defined over standard random variables

$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi)$$

$$R(\xi) \approx f(u)$$

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \, \Psi_j \, \varrho(\boldsymbol{\xi}) \, d\boldsymbol{\xi}$$

- Intrusive or non-intrusive
- Wiener-Askey Generalized PCE: optimal basis selection leads to exponential convergence of statistics

Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}$	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty,\infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	[-1, 1]
Beta	$\frac{(1-x)^{\alpha}(1+x)^{\beta}}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^{\alpha}(1+x)^{\beta}$	[-1,1]
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0,\infty]$
Gamma	$\frac{x^{\alpha}e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^{\alpha}e^{-x}$	$[0,\infty]$

Can also numerically generate basis orthogonal to empirical data (PDF/histogram)

Sample Designs to Form Polynomial Chaos or **Stochastic Collocation Expansions**



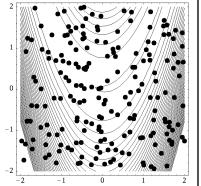
Random sampling: PCE

Expectation (sampling):

- Sample w/i distribution of x
- Compute expected value of product of R and each Y_i

Linear regression ("point collocation"):

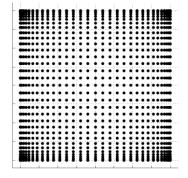
$$\Psi lpha = R$$



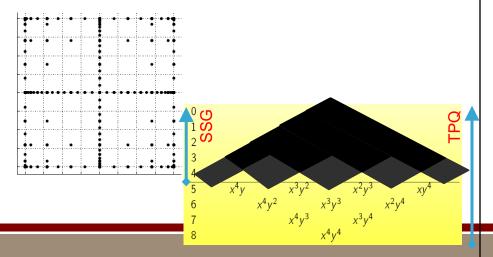
Tensor-product quadrature: PCE/SC

Tensor product of 1-D integration rules, e.g.,

Gaussian quadrature



Smolyak Sparse Grid: PCE/SC

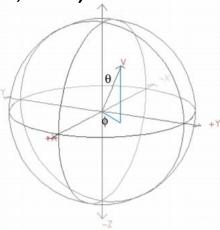


Cubature: PCE

Stroud and extensions (Xiu, Cools):

optimal multidimensional

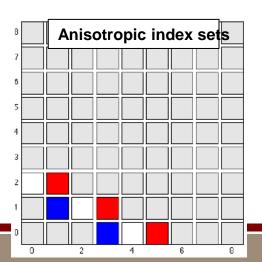
integration rules

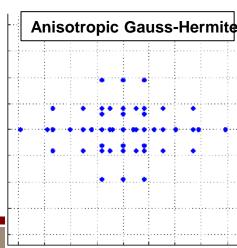


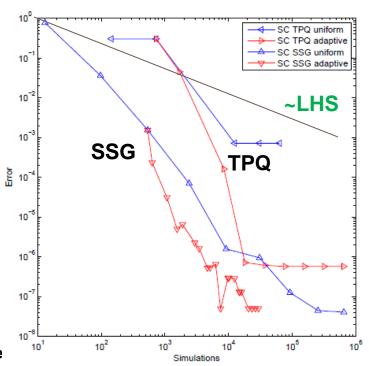
Adaptive PCE/SC: Emphasize Key Dimensions



- Judicious choice of new simulation runs
- Uniform p-refinement
 - Stabilize 2-norm of covariance
- Adaptive p-refinement
 - Estimate main effects/VBD to guide
- h-adaptive: identify important regions and address discontinuities
- h/p-adaptive: p for performance; h for robustness







Changes for Reliability, PCE



```
method,
     local reliability
      num probability levels = 17 17 17
       probability levels =
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
      .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
       cumulative distribution
responses
  response functions = 3
  descriptors = 'mass' 'stress' 'displacement'
  numerical gradients
    method source dakota
    interval type central
    fd gradient step size = 0.0001
no hessians
```

```
method,
    polynomial_chaos
    sparse_grid_level = 2
    sample_type lhs
    samples = 10000

    seed = 8572
    num_probability_levels = 17 17 17
    probability_levels =
        .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8

.85 .9 .95 .99 .999
        .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8

.85 .9 .95 .99 .999
        .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8

.85 .9 .95 .99 .999
        cumulative distribution
```

Uncertainty Quantification Research in Dakota: New algorithms bridge robustness/efficiency gap

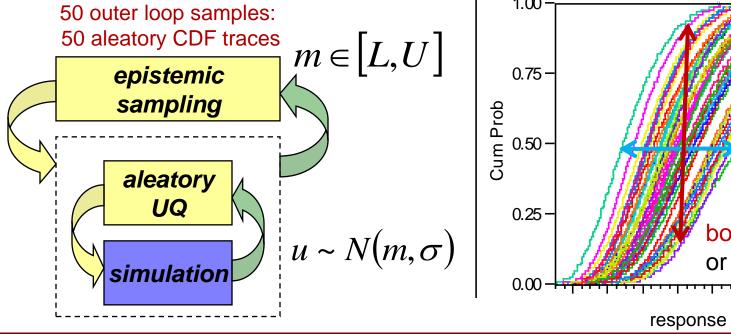


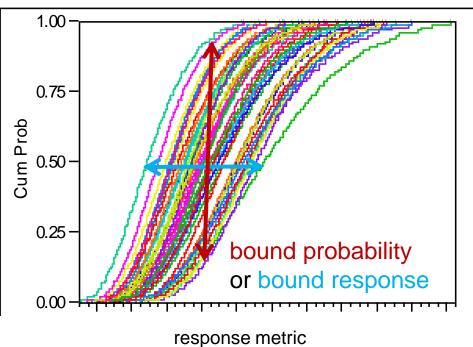
	Production	New	Under dev.	Planned	Collabs.
Sampling	Latin Hypercube, Monte Carlo	Importance, Incremental		Bootstrap, Jackknife	FSU
Reliability	Local: Mean Value, First-order & second-order	Global: Efficient global reliability analysis (EGRA)	gradient- enhanced	recursive emulation, TGP	Local: Notre Dame, Global:
	reliability methods (FORM, SORM)	Research: Adaptiv	Vanderbilt		
Stochastic expansion	Adv. Deployment Fills Gaps	PCE and SC with uniform & dimension-adaptive p-/h-refinement	Local adapt refinement, gradient-enhanced, compr sens	Discrete rv, orthogonal least interp.	Stanford, Purdue
Other probabilistic			Rand fields/ stoch proc	Dimension reduction	Cornell, Maryland
Epistemic	Interval-valued/ Second-order prob. (nested sampling)	Opt-based interval estimation, Dempster-Shafer	Bayesian, discrete/ model form	Imprecise probability	LANL, UT Austin
Metrics & Global SA	Importance factors, Partial correlations	Main effects, Variance-based decomposition		Stepwise regression	LANL

Aleatory/Epistemic UQ: Nested ("Second-order")Approaches



- Propagate over epistemic and aleatory uncertainty, e.g., UQ with bounds on the mean of a normal distribution (hyper-parameters)
- Typical in regulatory analyses (e.g., NRC, WIPP)
- Outer loop: epistemic (interval) variables, inner loop UQ over aleatory (probability) variables; potentially costly, not conservative
- If treating epistemic as uniform, do not analyze probabilistically!





Dakota Mixed UQ with Nested Model



- Two models, each with a different set of variables
- Outer method operates on nested model
- Inner method operates on simulation model

```
epistemic sampling

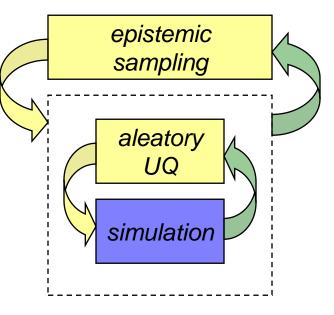
aleatory sampling

simulation
```

```
method
  id method = 'EPISTEMIC'
 model pointer = 'EPIST M'
  sampling sample type lhs
  samples = 5 seed = 12347
model,
  id model = 'EPIST M'
  nested
  variables pointer = 'EPIST V'
  sub method pointer = 'ALEATORY'
  responses pointer = 'EPIST R'
 primary variable mapping
                             = 'X'
  secondary variable mapping = 'mean' 'mean'
 primary response mapping = 1. 0. 0. 0. 0. 0. 0. 0. 0.
                               0. 0. 0. 0. 1. 0. 0. 0. 0.
                               0. 0. 0. 0. 0. 0. 0. 1.
variables,
  id variables = 'EPIST V'
  interval uncertain = 2
 num intervals = 1 1
  interval probabilities = 1.0 1.0
 upper bounds = 600.
                       1200.
  lower bounds = 400. 800.
responses,
  id responses = 'EPIST R'
  response functions = 3
  descriptors ='mean mass' '95th perc stress''95th perc disp'
 no gradients no hessians
```

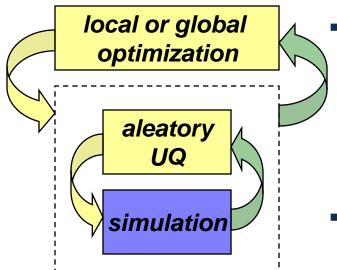
Example Output: Intervals on Statistics





Interval Estimation Approach (Probability Bounds Analysis)





- Propagate intervals through simulation code
- Outer loop: determine interval on statistics, e.g., mean, variance
 - global optimization problem: find max/min of statistic of interest, given bound constrained interval variables
 - use EGO to solve 2 optimization problems with essentially one Gaussian process surrogate
- Inner loop: Use sampling, PCE, etc., to determine the CDFs or moments with respect to the aleatory variables

$$\min_{u_E} f_{STAT}(u_A | u_E)$$

$$u_{LB} \le u_E \le u_{UB}$$

$$u_A \sim F(u_A; u_E)$$

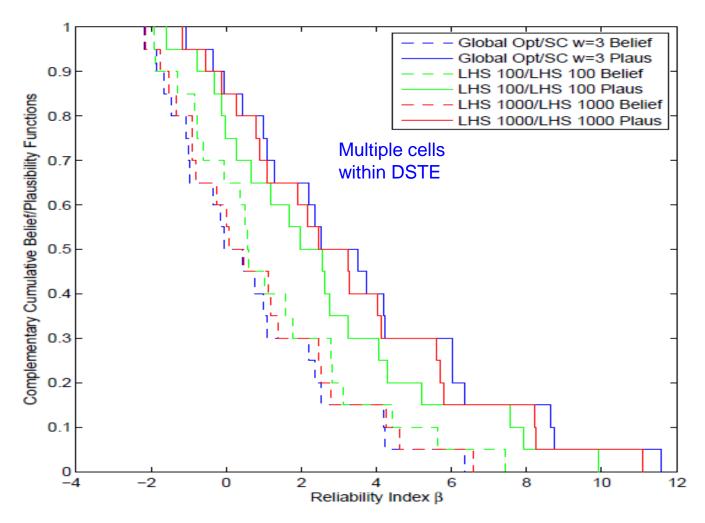
$$\max_{u_E} f_{STAT}(u_A | u_E)$$

$$u_{LB} \le u_E \le u_{UB}$$

$$u_A \sim F(u_A; u_E)$$

Interval Analysis can be Tractable for Large-Scale Apps





Converge to more conservative bounds with 10—100x less evaluations

Model Form UQ in Fluid/Structure Interactions



Discrete model choices for same physics:

- A clear hierarchy of fidelity (low to high)
- An ensemble of models that are all credible (lacking a clear preference structure)
 - With data: Bayesian model selection
 - Without data: epistemic model form uncertainty propagation

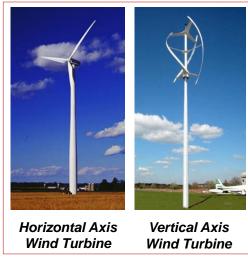
SA-RANS KE-RANS-NBC KE-RANS-DBC

Combination: Potential flow Vortex lattice

SA-RANS KE-RANS-NBC KE-RANS-DBC

Smagorinsky-LES Germano-LES

DNS



Low

Med

High

wind turbine applications

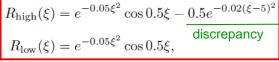
Multifidelity UQ using Stochastic Expansions 🕛

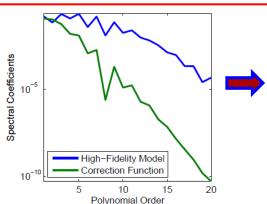


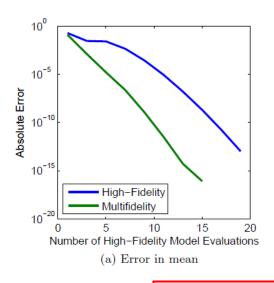
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

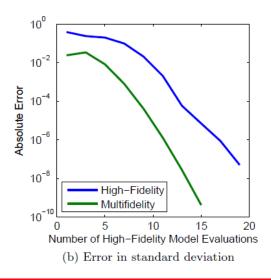
$$\hat{f}_{hi}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

$$N_{lo} >> N_{hi}$$









Low fidelity

CACTUS: Code for Axial and Crossflow TUrbine Simulation

High fidelity: DG formulation for LES Full Computational Fluid Dynamics/ Fluid-Structure Interaction

Uncertainty Quantification not Addressed Here



- Efficient epistemic UQ [Dakota]
- Fuzzy sets (Zadeh)
- Imprecise Probability (Walley)
- Dempster-Shafer Theory of Evidence (Klir, Oberkampf, Ferson) [Dakota]
- Possibility theory (Joslyn)
- Probability bounds analysis (p-boxes)
- Info-gap analysis (Ben-Haim)
- Bayesian model calibration / inference via MCMC [Dakota]
- Other Bayesian approaches: Bayesian belief networks, Bayesian updating, Robust Bayes, etc.
- Scenario evaluation

(Some available in [Dakota])

Dakota UQ: Summary, Relevant Methods



- What? Understand code output uncertainty / variability
- Why? Risk-informed decisions with variability, possible outcomes
- How? What Dakota methods are relevant?

character	method class	problem character	variants
aleatory	probabilistic sampling	nonsmooth, multimodal, modest cost, # variables	Monte Carlo, LHS, importance
	local reliability	smooth, unimodal, more variables, failure modes	mean value and MPP, FORM/SORM,
	global reliability	nonsmooth, multimodal, low dimensional	EGRA
	stochastic expansions	nonsmooth, multimodal, low dimension	polynomial chaos, stochastic collocation
epistemic	interval estimation	simple intervals	global/local optim, sampling
	evidence theory	belief structures	global/local evidence
both	nested UQ	mixed aleatory / epistemic	nested

- See Dakota Usage Guidelines in User's Manual
- Analyze tabular output with third-party statistics packages

UQ References



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- Helton, JC, JD Johnson, CJ Sallaberry, and CB Storlie. "Survey of Sampling-Based Methods for Uncertainty and Sensitivity Analysis", Reliability Engineering and System Safety 91 (2006) pp. 1175-1209
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- Haldar, A. and S. Mahadevan. Probability, Reliability, and Statistical Methods in Engineering Design (Chapters 7-8). Wiley, 2000.
- Eldred, M.S., "Recent Advances in Non-Intrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design," paper AIAA-2009-2274 in Proceedings of the 11th AIAA Non-Deterministic Approaches Conference, Palm Springs, CA, May 4-7, 2009.
- Dakota User's Manual: Uncertainty Quantification Capabilities
- Dakota Theory Manual
- Corresponding Reference Manual sections